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MODELING OF FUEL-AIR DETONATIONS:
THE DISTRIBUTED BLAST CONCEPT

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EXPERIMENTAL AND THEORETICAL MODELING OF FUEL-AIR
DETONATIONS: THE DISTRIBUTED BLAST CONCEPTDRS. NORMAN SLAGG, PAI-LIEN LU, BARRY FISHBURN
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INTRODUCTION

When an adequate (but relatively low) peak pressure is achieved, the destruction of certain types of military targets is determined by the total impulse generated by an explosive rather than by the brisance at a high peak pressure. Condensed (solid) explosives emphasize the achievement of high brisance; however, it has long been known that many heterogeneous dispersions of energetic substances in a medium can generate larger total impulses. If the substance is widely dispersed prior to initiation, such mixtures are effective over very large areas. Among Army explosive scientists the phenomenon has been identified as the distributed blast concept.

Unfortunately, the theoretical and experimental foundations for the concept are not well established. In this paper we present an analysis of results obtained in developing experimental techniques, defining critical explosive parameters and evolving a theoretical model for heterogeneous detonation.

The dispersions may be of the fuel-air type, where maximum energy release per unit volume is limited by the oxygen available in the atmosphere, or of the monopropellant type, where no external oxygen is required. Alternatively, the explosive may exist as a film on a surface (adjacent to the oxidizer gas in the fuel-air type). Most studies have centered on the detonation of clouds of liquid fuel drops in air.

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Experimental and theoretical studies have been performed to determine the interrelationships between chemical and physical factors in the ignition of liquid fuel drops by shock waves. It has been found that the mode of ignition of a drop may change with incident shock strength. A theoretical model has been developed to describe the complex process by which large liquid drops are fragmented. Theoretical comparisons are presented of the pressure and impulses generated by fuel-air clouds of different geometries and those from high explosives of equivalent weight and energy. In addition other types of heterogeneous detonation are considered. They include the use of solid fuel and film detonations.

THEORETICAL BASIS FOR DISTRIBUTED BLAST CONCEPT

Fig. 1 illustrates the propagation of a detonation through a fuel-air cloud. Upon reaching the edge of the cloud the detonation ceases and a blast (shock) wave propagates into the surrounding air. The curvature of the detonation is due to rarefaction waves which reduce the strength of the detonation wave by altering the flow. It is the shock waves associated with the detonation and blast that are capable of causing damage. We can generalize this phenomena by introducing the concept of "distributed blast." A "distributed blast" wave is generated from detonation in a dispersed explosive.

The advantage of fuel-air explosives arise from their utilization of atmospheric oxygen to produce a significant increase in the energy yield per unit weight carried and the fact that they are distributed. In Figs. 2 and 3 the theoretical pressures and impulses from gaseous ethylene oxide-air explosives are compared with the experimental outputs from conventional explosives. We calculated blast outputs using a modified version of a computer program developed by Oppenheim et al., based on the artificial viscosity method developed by von Neumann and Richtmyer.¹ The plots in Figs. 2 and 3 of pressure and impulse vs. radius clearly show the benefits of fuel-air explosives. Ethylene oxide and MAPP (Methylacetylene, propadiene, propane) are fuels being considered for munitions. MAPP gives more energy per unit weight than ethylene oxide upon reaction with atmospheric oxygen.

Changing the shape of the cloud from spherical to cylindrical, yields higher impulses. (Fig. 3) Thus another advantage of fuel-air explosives becomes evident. The pressure and impulse profiles can be varied by altering the cloud geometry. It is also seen that for equal energies of fuel-air explosive and pentolite, greater impulses can be

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obtained with fuel-air explosives at the sacrifice of peak pressures. It is to be recalled here that since fuel-air explosives have higher energy yields per unit weight, significantly less weight has to be carried to obtain an equivalent energy.

The available energy of a fuel-air explosive may not be realized due to the rarefaction wave (Fig. 1) which can alter the flow field and thereby remove energy from the blast or detonation wave. At present, theoretical calculations cannot be performed taking this factor into consideration due to the lack of a realistic physical model. In addition, comparisons between calculations of theoretical outputs and experiments are difficult at this time because the fuel-oxidizer ratio as a function of location is not sufficiently defined. Only when the parameters of cloud geometry and stoichiometry are known can the validity of a theoretical model be tested.

ENERGY RELEASE AND DETONATION CHARACTERISTICS

Detonation Models

A detonation can be defined as a shock front coupled to a chemical reaction zone that travels at constant velocity. The energy from the chemical reaction zone maintains the shock front. According to the Chapman-Jouguet theory of detonations, the chemical reactions occur behind the shock front and are completed at the Chapman-Jouguet plane where the products are in thermodynamic equilibrium. Energy released beyond this plane cannot support the shock front. Whether or not all the available chemical energy is released depends on the rates of the reactions, and physical processes in the case of two-phase detonations. Two-phase detonation refer to the case where the fuel is either in the form of liquid drops or solid particles and the oxidizer is gaseous. At present the major interest is in the case of liquid drops since fuels like ethylene and propylene oxides are under serious consideration.

According to the Chapman-Jouguet theory, the detonation pressure is approximately equal to $P_{CJ} = 2\rho Q(k-1)$ where ρ is the initial density, Q the heat of reaction and k the ratio of heat capacities C_p/C_v of the products if all products are gaseous.² For the case of solid products a more complicated equation depending on the equation of state is derived. Thus, with solid products the heat of combustion is only a rough guide to the relative pressures. In the case of metals, oxide formation on the surface of particles may cause the reaction to become diffusion controlled and thereby slow down preventing all the available energy from supporting the detonation. In Table I it is seen that the potential energies in the form of heat of

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combustion are similar regardless of the physical state of the fuel.

Table I

Heat of Combustion Per Gram of Fuel

| Fuel | Heat of Combustion per Gram (kcal/gm) |
|---|--|
| AL (s) | 7.3 |
| Be (s) | 16.9 |
| B (s) | 14.1 |
| C (s) | 7.8 |
| Decaborane (s) | 15.7 |
| Pentaborane (l) | 16.1 |
| Mg (s) | 6.0 |
| Jet Fuel (JP-4) (l) | 10.3 |
| n - C ₃ H ₇ NO ₃ (g) | 4.2 |
| n - C ₄ H ₁₀ (g) | 11.0 |
| C ₂ H ₂ (g) | 11.5 |
| C ₂ H ₄ O (Ethylene Oxide)(g) | 5.9 |
| MAPP (g) | 15.4 |

Experimental Studies of Drop Behavior and Energy Release

The interplay between chemical and physical factors that control the breakup of the drop and consumption of the fuel in a detonation can be seen in Fig. 4. The sequence reveals that the drop first deforms, an explosive mixture consisting of fuel mist and the gaseous oxidizer accumulates in the wake of the drop and later an explosion occurs in the wake. The explosion or detonation front grows radially until the fuel-oxygen mixture cannot support the detonation; at this stage the shock front decouples from the combustion zone and propagates outwardly as a blast wave. As time increases the burning wake grows longitudinally.³ Obviously increasing interactions between drops will occur with increasing drop density. Since the behavior of the fuel drops determine the detonation properties, studies have been performed by us and other researchers in order to elucidate the relative importance of various parameters. The main thrust of our drop studies described below has been to determine the mechanism for mass stripping in the supersonic flow behind the incident shock wave, ignition delay times, and the strength of blast waves formed in the wake of drops.

Other researchers have been mainly concerned with hydrocarbon fuels and neglected the role of chemistry. Studies have been made by us on the following fuels to determine the role of chemistry in ignition of drops of nitromethane, 1 and 2 nitropropane, ethyl and propyl nitrates, nitrobenzene, butyl alcohol, heptane and decane. The experimental setup (Fig. 5) has been described elsewhere,³ and will only be briefly described here.

The time interval between signals from pressure transducers placed along the wall enabled us to calculate the average shock wave speed. A spark light source schlieren system was used to obtain a photographic record. The light pulse width was about 0.3 μ sec and was synchronized to the event by means of a time delay generator which in turn was triggered by the pressure transducer signal via the oscilloscope. In this manner schlieren photographs were obtained at different times after the shock passed over the drop. A photodiode via an oscilloscope was used to determine the luminosity which indicates onset of ignition.

Of all the fuels tested with an incident shock of Mach number 3.3 in pure oxygen only ethyl and propyl nitrate were observed to ignite and explode. It is interesting to compare the bond energies of fuels as shown in Table II.³

Table II
Bond Energies

| Molecule type* | Bond Energy (kcal/mole) |
|-------------------------|-------------------------|
| R-H | 85 - 100 |
| R-OH | 90 |
| R-NO ₂ | 58 |
| RO-NO ₂ | 37 |
| ϕ -NO ₂ | 70 (estimate) |

*R is an aliphatic radical, ϕ is the phenyl radical.

Since the nitrates have the weakest bond, the RO-NO₂ bond, they are expected to decompose at lower temperatures which suggests that the chemical bond strength is an important factor for ignition by shock wave.³ The ignition delay times (time for the observation of luminosity after the passage of the shock wave) are given for the various fuels as a function of incident shock strength in Fig. 6. In agreement with Kauffman et al., it was observed that the ignition delay time for large drops is longer than that for small drops.⁴

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The data suggests an exponential behavior as

$$t_{ig} \propto e^{\Delta E/RT}.$$

The ΔE is believed to be the net result of important physical and chemical processes. Fig. 6, illustrates that the nitrates have shorter ignition delay times compared with other fuels at the same incident shock strength. The physical properties that control the drop breakup are similar for the fuels tested.^{5,6} Thus, the difference in ignition delay data between nitrates and other fuels must be due to chemical factors.

Two interesting phenomena were observed at higher incident shock Mach numbers (above $M_s = 3.5$) with the nitrates: (1) burning occurred in the boundary layer prior to breakup of the drop; and (2) no blast wave was observed in the wake as seen in Fig. 7.⁵ Previous results by other workers were usually discussed in terms of the breakup time (the time for the drop velocity to become 60% of the convective velocity of the gas).⁴ A tacit assumption was being made that the shattering of the drop is required before the onset of chemical reactions. At least for the nitrates, it is seen that ignition can occur in so short a time that no appreciable wake formation is evident from the photographs. Thus shattering may not be necessary for ignition at sufficiently high incident shock Mach numbers.

The observation that blast waves do not occur in the wake of nitrate drops at higher incident shock strengths is consistent with the observation of ignition in the boundary layer. Since ignition occurs in the boundary layer region at a very short time ($\sim 7 \mu\text{sec}$), very little accumulation of fuel in the wake is expected. Therefore an explosive mixture is not formed and blast waves should be absent. Thus it appears that as one goes from low to higher Mach numbers, at least for the nitrates, there is a change in the mode of ignition. Additional efforts are required (1) to determine if other fuels at higher incident shock strengths will also undergo a change in mode of ignition, and (2) to clarify the mechanisms by which various fuels release their energy in support of the detonation.

Theoretical Studies

The drop deformation discussed in the previous section is a result of complex physical factors which affect the rate of energy release that sustains the shock front of the detonation. Studies were undertaken to clarify these various important physical processes. Analysis suggested that stripping of the liquid from the drop is due to

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shear forces from the high speed gas flow associated with the detonation.⁶ Mass stripping removes a 10-20 micron thick liquid layer from the drop, which is carried into the wake of the drop where a fuel mist is formed. Superposed on this process is the growth of disturbances on the unstable front surface of the drop and flattening of the drop by pressure applied by the gas (Fig. 8). The disturbances eventually shatter the drop into fragments, still large compared to the typical diameters in the mist. Mass stripping then proceeds much more rapidly due to the increased surface to volume ratio of these liquid fragments. Calculations based on this model compare favorably with mass loss data given by Reinecke and Waldman.⁷

These results show that the most important feature in the break-up process is shattering of the parent drop into fragments that are still large compared to diameters in the mist. The time after passage of the incident shock at which fragmentation occurs is basically determined by the time required for the drop to be flattened by the gas flow. In addition, this model indicates that shattering always occurs at about the same degree of drop deformation regardless of the Mach number or original diameter.

The blast waves observed in the wake of fuel drops merge to form the detonation. Thus it is necessary to perform theoretical studies to determine the nature of these blast waves and the extent to which the blast wave from one drop influences an adjacent drop. The energy driving these blast waves comes from the associated chemical reactions whose rates, in addition to depending on the usual factors such as temperature and pressure, also depend on the degree of shattering of the drop. Blast wave analysis of exploding drops by Dabora revealed, not surprisingly, that the blast wave does not originate from a point source with an instantaneous release of energy, which suggests a complex process for the energy release requiring further studies.⁸

OTHER TYPES OF HETEROGENEOUS DETONATIONS

As pointed out earlier the fuel can either be a gas, liquid, or solid. With regard to a solid fuel it should be realized that condensed explosives are also monopropellants, and that detonations may occur in dispersed explosives without the utilization of atmospheric oxygen. It is to be recalled here (see Fig. 3) that theoretical calculations suggest that a dispersed explosive may yield higher impulses than compact explosive of equivalent energy.

Solid Fuels

The interest in solid fuels stems from the ability to control particle size and ease of handling. Many studies have been performed to determine the hazards of flame and explosions from various dusts.^{9,10,11} The results indicate that explosions and/or detonations can occur in unconfined dust-air mixtures. It has been shown that dusts of Zr, Mg, Al, and Ti are capable of exploding in air. Furthermore, Mg and Zr dusts were found to be capable of exploding in nitrogen with only a few percent oxygen.⁹ Only two examples can be found in the literature for detonations in dispersions of solid particles in a gaseous oxidizer. The solids are aluminum and coal.^{12,13} Strauss demonstrated that aluminum particles-gaseous oxygen mixtures in a shock tube were capable of sustaining a detonation. The mixtures studied contained 48-64% by mass of aluminum. The mean diameter of a flaked aluminum sample was 40 μ , and the average diameter of a granular sample was 5 μ . Both samples sustained detonations that were approximately 10% below theoretical predications. The detonation pressure was about 31 atmospheres. Recent shock tube studies at Picatinny Arsenal strongly suggest that detonations can occur in mixtures of fine aluminum flakes and air.¹⁴ It is imperative that work of this type be pursued to determine if detonations can occur in unconfined solid fuel-air mixtures.

Film Detonation

Another type of detonation that can result in a distributed blast is detonation of a thin film of liquid fuel with a gaseous oxidizer above it. Gordeev et al. reported the first definitive study of film detonations for various liquid film-gaseous oxidizer combinations.¹⁵ Ignition of thin layers of lubrication oil, grease, and carbon black was accomplished by a $\text{CH}_4\text{-O}_2$ detonation, an exploding wire, and a charge of lead azide in a 22mm diameter tube. Kamov and Troshin studied the effect of mixture ratio and initial pressure on the detonation.¹⁶ Ragland and Nicholls demonstrated that a 10-20 μ layer of diethylcyclohexane, in an oxygen atmosphere, can sustain a detonation when the film is either on one or two walls of a rectangular shock tube.¹⁷ In another study it was shown that a thin layer of decane in a 30% oxygen atmosphere could detonate.¹⁸ Recent studies have shown that a wide variety of fuel film-air mixtures can detonate in tubes.¹⁹

A two dimensional theory has been developed by Rao, Sichel, and Nicholls.²⁰ Vaporization is believed to be the rate limiting process dominating the structure of the detonation. The Chapman-Jouguet plane is taken to be the point where vaporization of the film is complete. Incorporation of turbulent boundary layer losses give better agreement between theory and experiment. Work on unconfined film-air mixtures is

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required (which will be performed at Picatinny Arsenal in the near future) in order to assess the potential of this phenomena.

CONCLUSION

Our theoretical studies have revealed the wide range of blast outputs (pressure and impulse) that can be achieved by distributed explosives. The experimental efforts have indicated that fuel drops may have more than one mode of ignition, which is dependent on the incident shock strength. The more important physical parameters involved in the deformation and destruction of the fuel drops were clarified by the formulation of a theoretical model. Furthermore, a wide variety of heterogeneous detonations have been highlighted indicating the potential flexibility in munition design and delivery systems.

The major thrust in future efforts should be directed to establishing the relationships between rarefaction waves, cloud geometry, and the manner in which the fuel element, liquid or solid, is consumed.

Present munitions have demonstrated the value of the concept, yet we have just opened the door to a source of energy, as much as ten times greater per unit weight than conventional explosives.

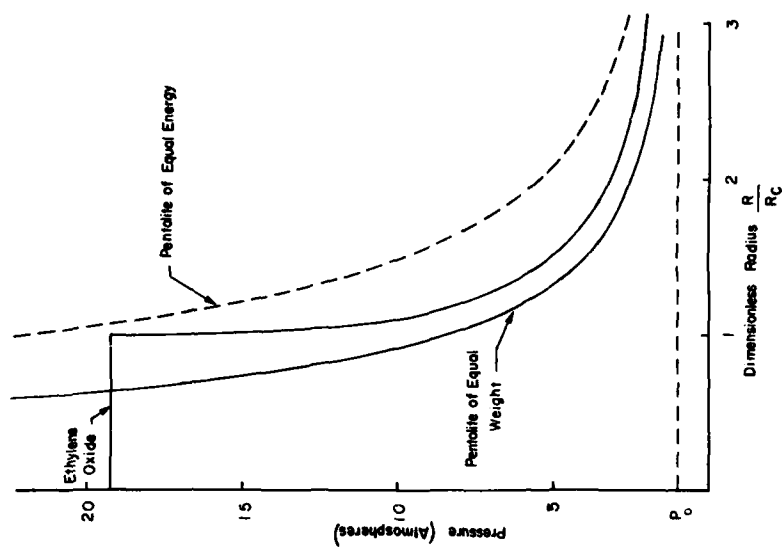


Figure 2. Peak Pressures Produced by Ethylene Oxide and Pentolite Detonations. (Cloud Radius = R_C)

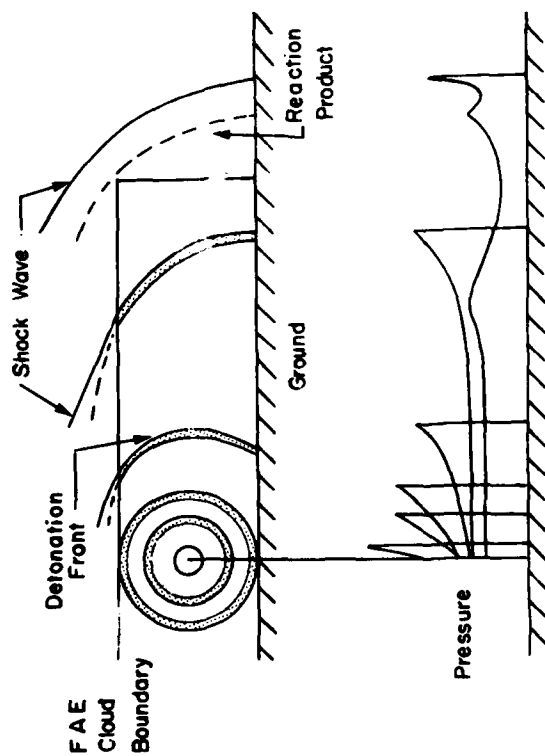


Figure 1. The Time Dependent Histories of the Detonation Wave Front Shape and Pressure.

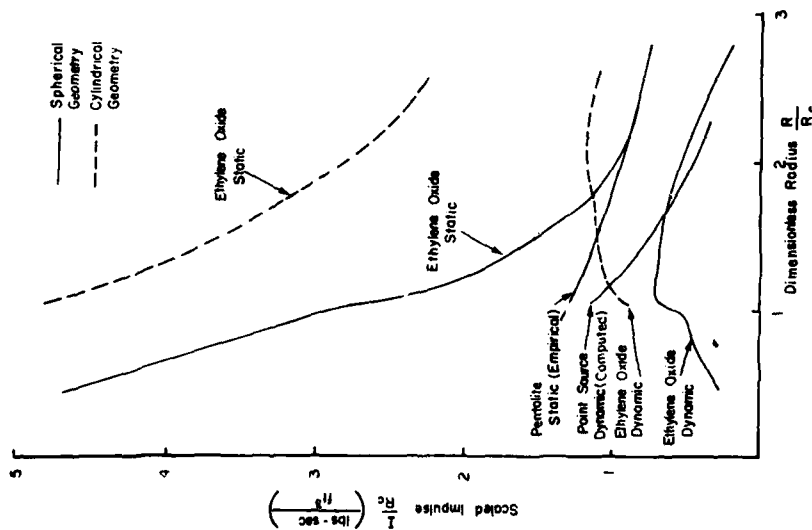


Figure 3. Impulses Produced by Detonations From Spherical and Cylindrical Clouds of Ethylene Oxide, Equivalent Energy of Pentolite and a Point Source. (Cloud Radius = R_c)

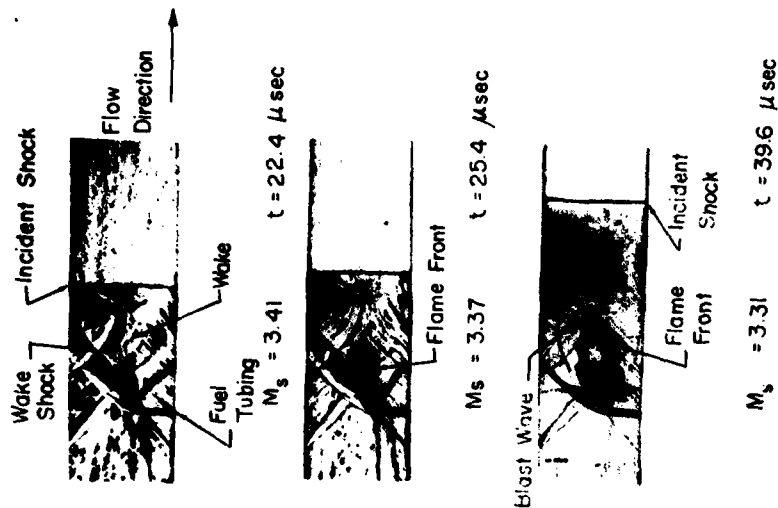


Figure 4. Shock Ignition of a Propyl Nitrate Drop in an Oxygen Atmosphere. (The Time Refers to the Interval Between the Incident Shock Striking the Drop and the Time Of the Photograph).

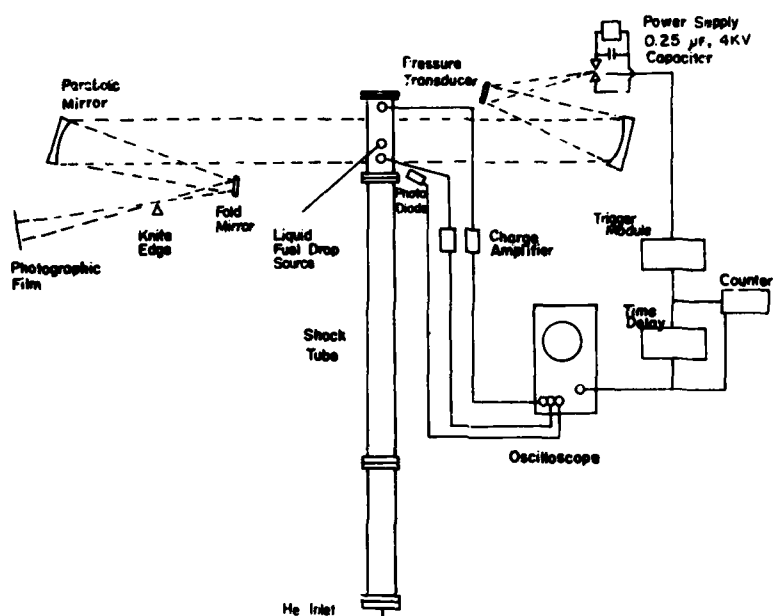


Figure 5. Schematic Diagram of the Shock Tube System.

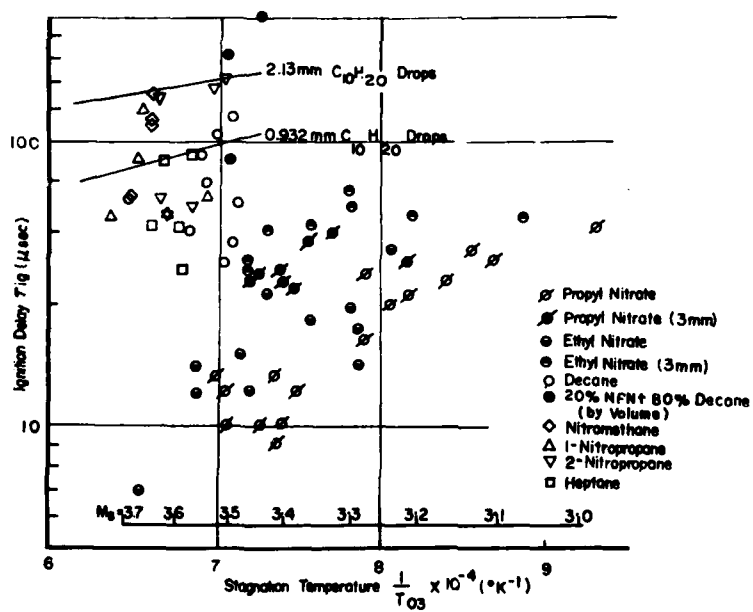


Figure 6. Ignition Delay Times for Various Fuels (Drop Size 1.69mm) in Oxygen.

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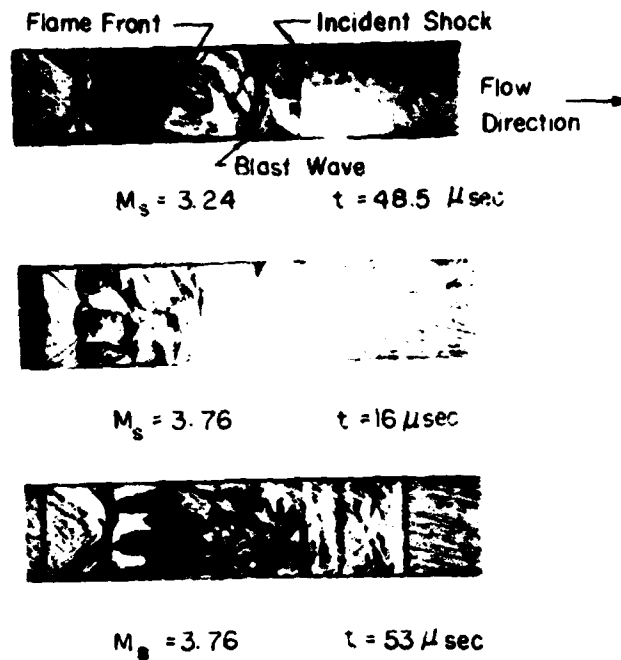


Figure 7. Effects of Incident Shock Mach Numbers on Ignition Mechanism of Propyl Nitrate Drops in Oxygen.

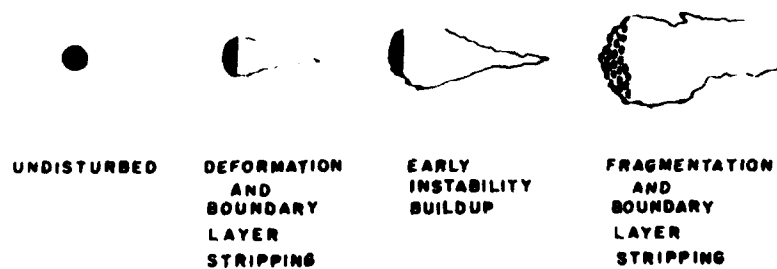


Figure 8. Phenomena Associated With Breakup of Fuel Drops in a Two Phase Detonation.

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